

Supporting Information

Kinetics and Stereochemistry of Hydrolysis of a N-(Phenylacetyl)- α -Hydroxyglycine Ester Catalyzed by Serine β -Lactamases and DD-Peptidases

Ryan B. Pelto and R. F. Pratt

Department of Chemistry, Wesleyan University, Lawn Ave., Middletown, CT 06459, USA. E-mail: rpratt@wesleyan.edu

Figure S1. ^1H NMR spectrum of **5**.

Figure S2. HPLC of **5**.

Figure S3. Reaction of PAL with the TEM products.

Figure S4. ^1H NMR spectrum of **5** in phosphate buffer: spontaneous reaction.

Figure S5. ^1H NMR spectrum of **5** in phosphate buffer: spontaneous reaction products.

Figure S6: ^1H NMR spectrum of **5** in phosphate buffer: spontaneous reaction products and non-products.

Figure S7. ^1H NMR spectrum of **6** in phosphate buffer.

Figure S8. ^1H NMR spectrum of **5** in phosphate buffer: products from reaction with P99 β -lactamase.

Figure S1. ^1H NMR spectrum of **5** in $\text{D}_6\text{-DMSO}$

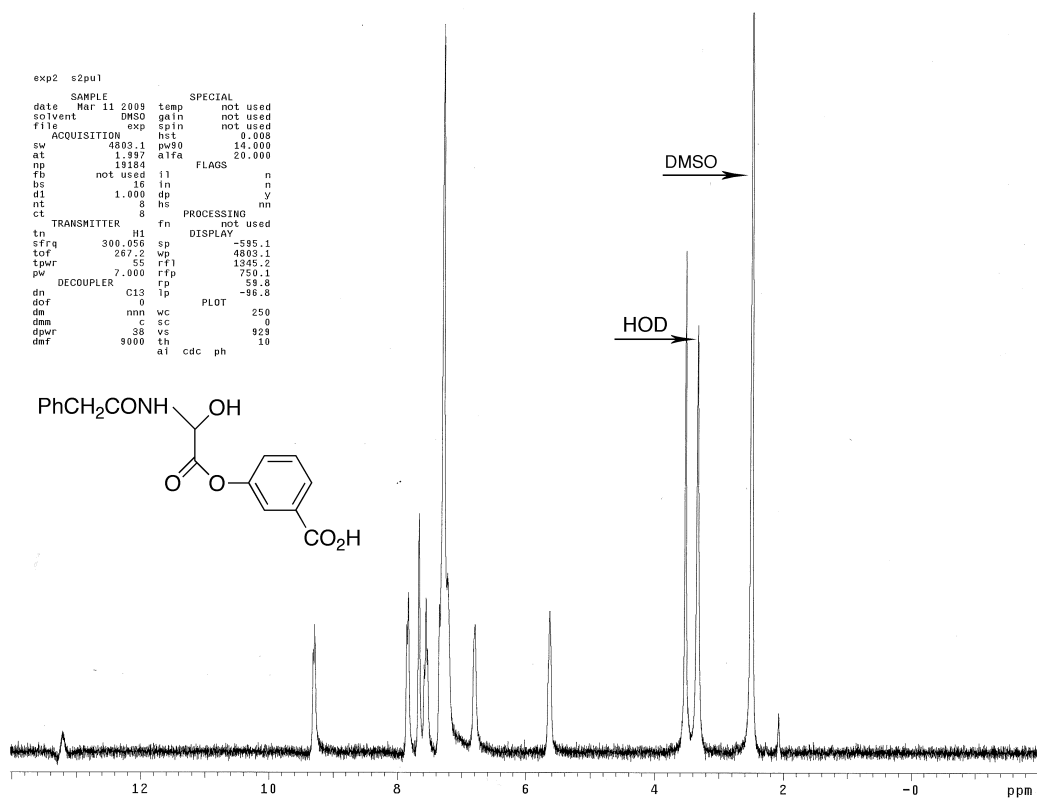


Figure S2. HPLC chromatogram of **5**

Reverse phase C18 HPLC chromatogram of **5** (mobile phase 80% phosphate, 20% methanol, pH 7.5). Absorption recorded at 258 nm.

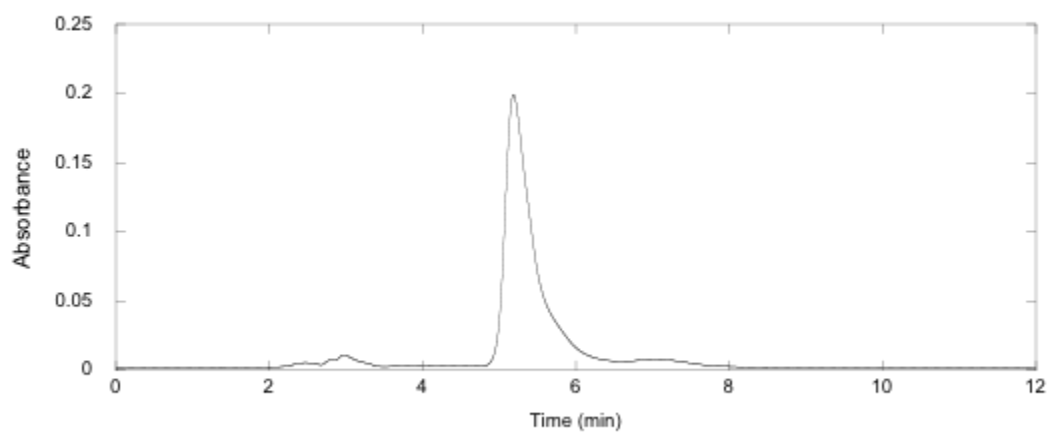


Figure S3. HPLC traces from the reaction of PAL with the products of the reactions of **5** in the presence of the TEM β -lactamase, carried out as described in the main text.

Reverse phase C18 HPLC chromatograms of aliquots taken at suitable times from the reaction mixture (mobile phase 80% phosphate, 10% methanol, pH 7.5, absorption recorded at 258 nm). The various traces show the disappearance of L(S)-**5** (9.0 min) by spontaneous hydrolysis and the accompanying appearance of phenylacetamide (6.9 min) and *m*-hydroxybenzoate (2.9 min). Also present is D(R)-**6** (3.8 min) and *m*-hydroxybenzoate from the β -lactamase reaction.

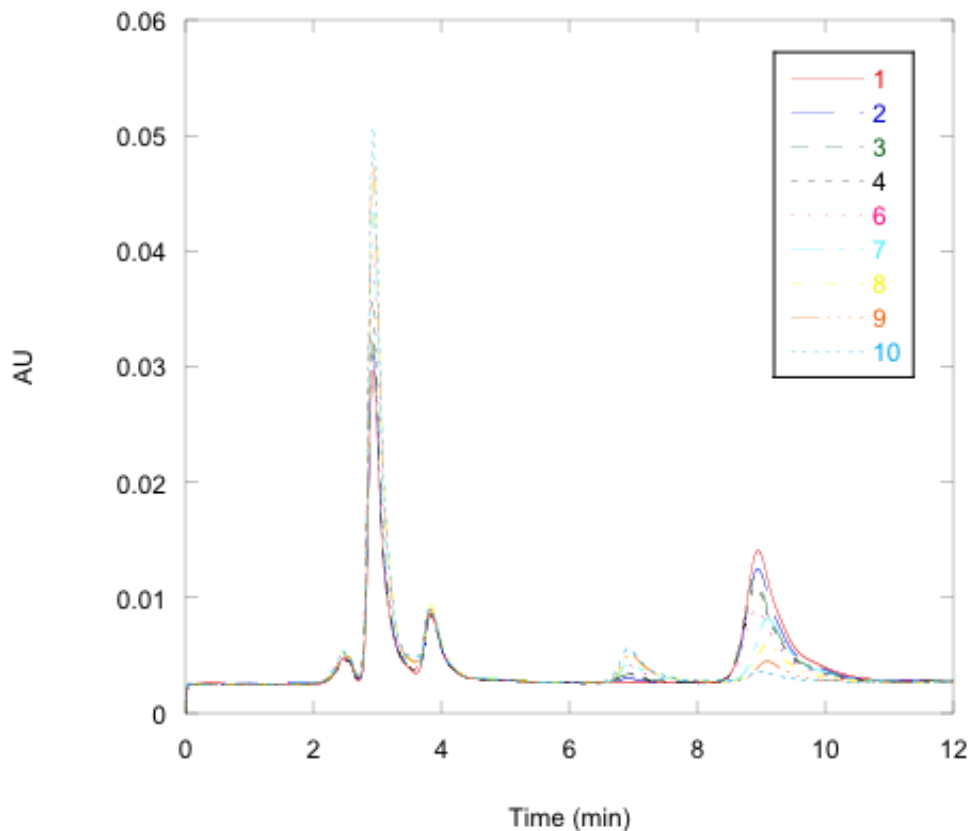


Figure S4.

^1H NMR spectrum of **5** (2.4 mM) in phosphate buffer (13 mM), pH 7.5. Small amounts of the spontaneous hydrolysis products are also seen (see spectra below).

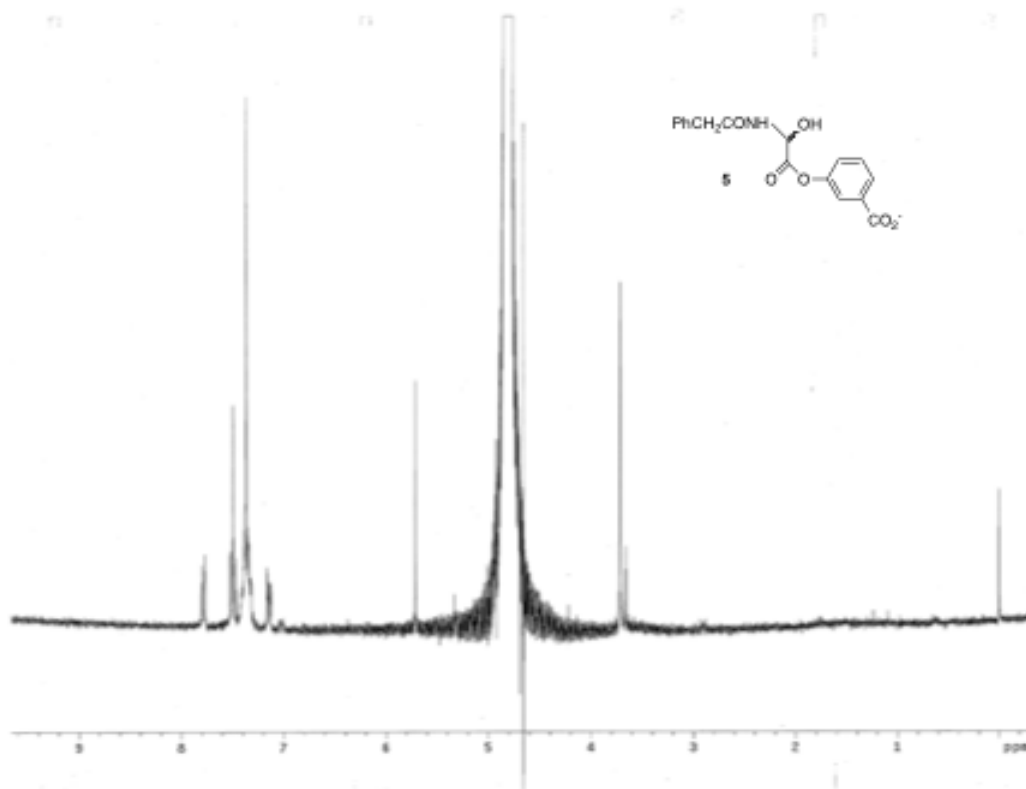


Figure S5.

^1H NMR spectrum of **5** (2.4 mM) in phosphate buffer (13 mM), pH 7.5, after its spontaneous hydrolysis to **6** is almost complete. A small peak from a bimolecular side reaction is also seen at δ 6.0.

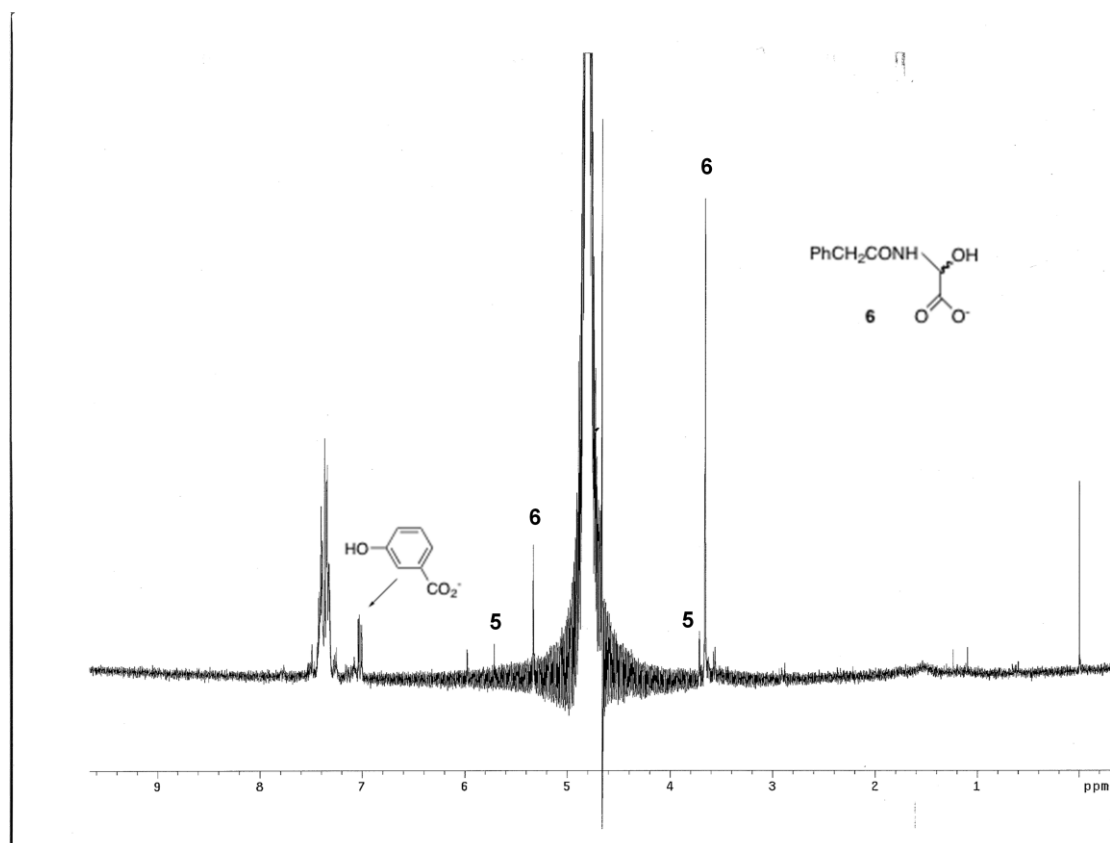


Figure S6.

A ^1H NMR spectrum of the final solution from the reaction of Figure S5, after addition of authentic samples of glyoxylic acid and phenylacetamide to it.

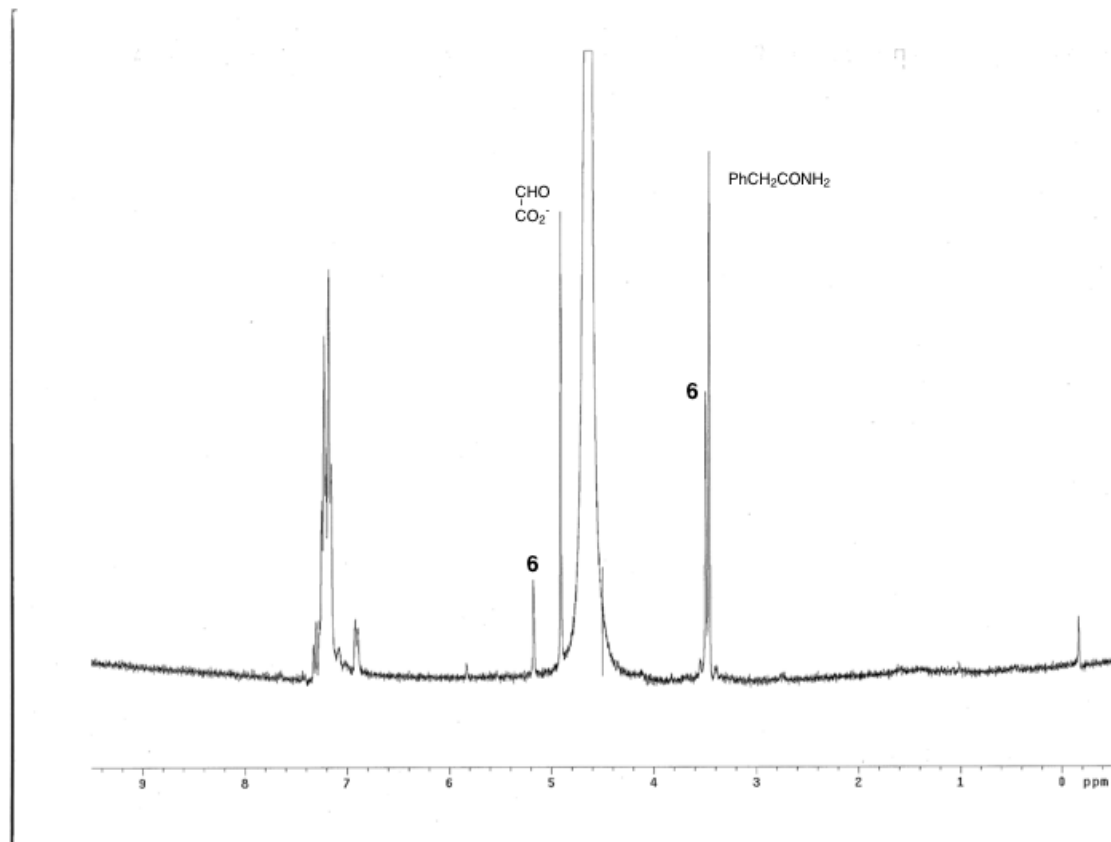


Figure S7.

^1H NMR spectrum of authentic **6** in phosphate buffer as above. The compound was stable under these conditions for at least 24 hr.

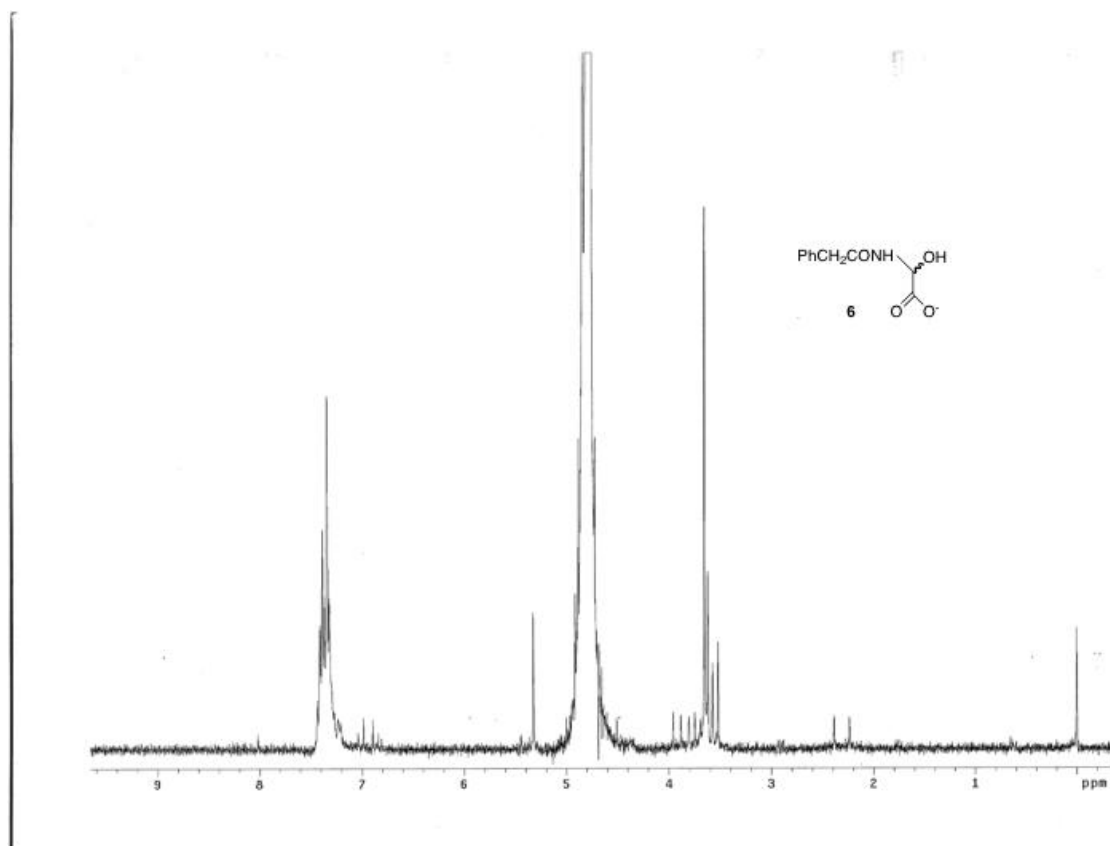


Figure S8.

^1H NMR spectrum of a solution of **5** in phosphate buffer, as above, 15 min after addition of the P99 β -lactamase (ca. 100 μg). Both enantiomers of **5** are substrates of this enzyme (see main text).

